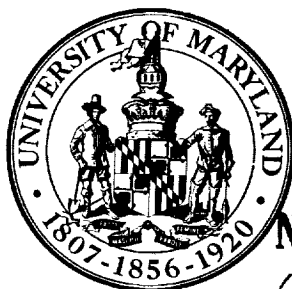


UNPUBLISHED PRELIMINARY DATA

NSG-5-59

CR-50,453

UNIVERSITY OF MARYLAND



N 63 18321

Code-1

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IMP-NASA-33

June 17, 1963

INTERACTION ENERGIES AND TRANSPORT COEFFICIENTS OF
Li + H AND O + H GAS MIXTURES AT HIGH TEMPERATURES*†

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ABSTRACT

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Accurate potential energy curves for the $X^1\Sigma_g^+$, $A^1\Sigma_u^+$, $B^1\Pi_u$, and $C^1\Pi_u$ states of the Li_2 molecule are calculated from observed spectroscopic data by the method of Rydberg-Klein-Rees (RKR), and compared with previous quantum-mechanical calculations. Long-range attractive potentials are estimated by extrapolation of functions fitted to the RKR ground-state curves of Li_2 , LiH , and OH . From these, the repulsive potentials derivable from interacting ground-state atoms are estimated semiempirically. Collision integrals computed from the potentials, and transport coefficients of the gaseous systems $Li + Li$, $Li + H$, and $O + H$ are calculated for temperatures of 1000 to 10 000°K.

A surprising result is the extraordinarily large values of the collision integrals for $Li + Li$ (and $Li + H$) interactions, which result in unexpectedly small values of diffusion coefficient, viscosity, and thermal conductivity. For traces of Li in $Li + H$

*Based in part on a thesis submitted by P.H.K. to the Department of Physics, University of Maryland, in partial fulfillment of the requirements for the degree of Master of Science.

†Supported in part by the National Aeronautics and Space Administration (Grant NsG-5-59).

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mixtures at low temperature, the thermal diffusion factor is very large. Various approximate formulas for viscosity and thermal conductivity of mixtures are seen to give poor agreement with exact calculations for the systems considered.

I. INTRODUCTION

The present paper is one of a series on the calculation of high-temperature transport properties of gases.^{1,2} Here we consider the gaseous systems Li + Li and mixtures of Li + H and O + H in the temperature range of 1000 to 10,000°K. Li + Li and Li + H interactions are of fundamental interest because of their relative simplicity. OH is a constituent in stellar atmospheres and is often the subject of study in flames; hence the importance of the O + H interactions. At one atmosphere pressure, Li₂ is 95% dissociated at 2000°K; Li ions become important at 6000°K. For Li + H mixtures,³ molecules constitute less than 5% of the system at 1500°K, and ionization reaches 5% at 6000°K. For O + H mixtures,⁴ dissociation is about 95% complete at 4000°K, and at 10,000°K, ions constitute only about 2% of the system. Since atoms are the dominant species throughout most of the temperature range under consideration, only atom-atom interactions are included.

The expressions for the transport coefficients, given previously,¹ are in terms of collision integrals, which are complicated functions of the interaction potentials. Thus, the problem of calculating transport coefficients reduces to one of determining

the interaction potentials. Only potentials derivable from interacting ground-state atoms are considered. The potentials are estimated from a combination of approximate quantum-mechanical expressions and extrapolations of experimental potentials obtained from spectroscopic observations by the method of Rydberg-Klein-Rees.⁵⁻⁷ The latter method is a well-established means of determining potential curves over a range of internuclear separations determined by the spectroscopic data.⁸ The transport coefficients are calculated in terms of collision integrals which are obtained by curve-fitting the potentials with functions for which collision integrals have been tabulated.

II. CALCULATION OF THE POTENTIAL CURVES FOR Li_2

The potential energy curves for the $X^1\Sigma_g^+$, $A^1\Sigma_u^+$, $B^1\Pi_u$, and $C^1\Pi_u$ states of Li_2 were calculated by the method of Rydberg-Klein-Rees.⁵⁻⁷ In the calculations, we have used the spectroscopic data of Loomis and Nusbaum,⁹ McKellar and Jenkins,¹⁰ Harvey and Jenkins,¹¹ Wurm,¹² McKellar,¹³ Barrow, Travis, and Wright,¹⁴ and unpublished data of Barrow.¹⁵ Barrow concludes from the rotational analysis of the strong C-X bands in the UV that the C state should be $^1\Pi_u$ and not $^1\Sigma_u^+$ as listed in Herzberg.¹⁶

The vibrational energy levels and turning points of the observed states are listed in Tables I to IV, and are shown also in Fig. 1. Several quantum-mechanical calculations of potential curves for Li_2 have been reported. Ishiguro, et al.¹⁷ give binding energies for the $X^1\Sigma_g^+$, $^3\Sigma_u^+$, $A^1\Sigma_u^+$, and $B^1\Pi_u$ states

which differ from the observed by about a factor of two. Besides the above states, Fraga and Ransil¹⁸ include the $^3\Sigma_u^+$, which crosses the ground state (but shouldn't), and $^1\Sigma_u^+$ which falls too high by about 0.7 ev. Their curve for the ground state is very good, but begins to bend too sharply upward at about 4\AA^0 . Fieschi¹⁹ gives vertical excitation energies from the ground state to the A and B states. Except for the data of Fraga and Ransil¹⁸ the other calculations are for isolated points. The calculated data are neither extensive enough nor sufficiently accurate to require graphical comparison at this time with the RKR curves.

III. ESTIMATION OF LONG-RANGE ATTRACTIVE AND REPULSIVE POTENTIALS

In the cases studied here, direct experimental potentials for large internuclear separations are not available, and the theoretically calculated curves do not reproduce the experimental curves where available, and are considered unreliable. We must then rely on semiempirical functions to be used in a more critical fashion than just being fitted to the spectroscopic constants, by selecting that function which best fits the RKR potential. The best one can do at the present is to extrapolate such functions into the region of interest. In addition, the real potential is assumed not to change form with increasing internuclear separation. That this may not strictly be the case is illustrated by the behavior of the B state of Li_2 ,⁹ where, at vibrational quantum number 12, there is an abrupt change in the spectroscopic constants which fit the experimental energy levels (indicating a change in the force law).

The RKR ground states of Li_2 , LiH , and OH were fitted by semiempirical functions for the purpose of extrapolating to long range. The state for Li_2 was that given in Table I. The curve for LiH was taken from ref. 20, and that for OH from ref. 8. The following functions were considered: Morse, Lippincott 5-parameter, Rydberg, and Varshni^{#3}.²¹ As written here, the zero reference is at the bottom of the potential well. For the ground state of Li_2 a number of values for the dissociation energy (D_0) have been reported, ranging from 1.03 to 1.14 ev. A compromise value of 1.12 ev was chosen, based on the brief discussion of Evans²² et al. This gives a D_e of 1.14 ev (9195 cm^{-1}).

Once the semiempirical function was obtained, the method of Hirschfelder and Eliason²³ was used to determine the internuclear distance interval over which the extrapolated function was to be fitted by a potential for which collision integrals have been tabulated. [Hirschfelder and Eliason show that only the region of the potential energy function near $U(r) \sim kT$ is important in determining transport coefficients at temperature T . Essentially, they use an inverse power function to obtain effective rigid sphere diameters corresponding to a given temperature and property. This parameter determines the region (r interval) that must be fitted.] For a discussion of the method see the paper on hydrogen.¹ An exponential function was fitted to the extrapolated functions by least-squares in all cases considered here, including the repulsive curves discussed below, with deviations of only a few percent.

The attractive potentials were obtained from the RKR

potentials in the manner discussed. Curves for the $^3\Sigma$ states of both Li_2 and LiH were estimated by a method given by Keyes,²⁴ with effectively, a reversal in the sign of the exchange effect term in the semiempirical functions fitted to the RKR curves. This was done using a Morse²¹ and Lippincott²¹ function for Li_2 , and a Varshni²¹ function for LiH . For OH the matter is complicated because, from the Wigner-Witmer rules,²⁵ the $^2\Pi$ ground state as well as $^2\Sigma^-$, $^4\Pi$ and $^4\Sigma^-$ states arise from interaction between ground state O and H atoms. This will be discussed in the next section.

As a rough guide to the uncertainties involved in using these semiempirical procedures, a comparison was made between approximate and accurately known curves for hydrogen.^{21,26} The accurate RKR curve for the ground state was compared with a fitted Lippincott function, and the lowest $^3\Sigma_u^+$ repulsive state, calculated by Dalgarno and Lynn,^{26b} was compared with a Rydberg²¹ function fitted to the ground state, and modified to predict the repulsive state by the method of Keyes. The approximate curve for the attractive state fell below the accurate curve by 10 - 50%. The estimated repulsive curve lay higher than the accurate curve by a factor of 2 - 4. Greatest uncertainties, in both cases, were for longer range. The effect on the transport coefficients is discussed in the concluding section.

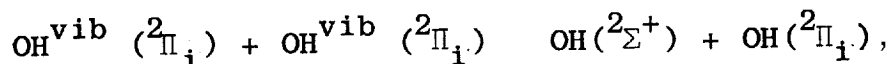
IV. POTENTIAL CURVES FOR OH

The Wigner-Witmer rules²⁵ determine the possible molecular electronic states that arise from the interaction of atoms in specified states (in this case, $\text{O}(^3\text{P}) + \text{H}(^2\text{S})$). The molecular states for OH

include ${}^2\Pi_1$ (ground state), ${}^2\Sigma^-$, ${}^4\Pi$, and ${}^4\Sigma^-$. The RKR potential for the ground state⁸ of OH was fitted by a Lippincott 5-parameter function,^{21b} and the methods described previously were employed to obtain the extrapolated attractive curve used in calculating collision integrals. The general conclusion drawn regarding the excited states is that there is not sufficient theoretical or experimental evidence to specify their curves accurately. To estimate the position of these states, the simplified Heitler-London theory was used. A brief review of what is known about these states is in order before going on to a discussion of the application of the Heitler-London theory.

Fallon, et al.⁸ discuss the experimental evidence which indicates that the ${}^2\Sigma^-$ state predissociates the A ${}^2\Sigma^+$ state at the $v = 2$ level, and also discuss Mulliken's²⁷ prediction that the three excited states are all repulsive, which indicates the ${}^4\Pi$ as most likely causing the predissociation. Either of these choices appears to violate the Kronig selection rules.²⁸

Michel²⁹ refers to a sudden drop in intensity of all rotational lines with $K \geq 6$ of the 0-8 band of the $C \rightarrow A$ and $B \rightarrow A$ systems. Since the 0-7 and 0-6 bands have regular intensity distribution, this indicates a predissociation of the eighth vibrational level in the A ${}^2\Sigma^+$ state. Michel ascribes the predissociation to the ${}^4\Pi$ state. Broida³⁰ suggests that the conversion of vibrational energy to electronic energy accounts for the excess excitation in lower vibrational levels of the A state through the reaction:



but does not specify which vibrational levels in the A state would be affected. He asserts, however, that for colliding molecules with combinations such that $v_1 + v_2 \geq 10$, such collisions should rather efficiently populate the A state.

The Heitler-London expressions for the lower states of OH have already been given by Stehn.³¹ These energy expressions can be written as a sum of coulombic and exchange terms if the appropriate overlap integrals are neglected.³² At larger values of r , the coulombic terms are much smaller than the exchange terms.^{33,34} Further, multiple exchange terms are usually much smaller than single exchange terms. If we neglect both these coulombic and multiple exchange terms, Stehn's energy expressions for the states of interest reduce to those given in Table 5. Here J_σ refers to the exchange integral involving the H 1s and the O 2p σ , and J_π refers to the exchange integral involving the H 1s and the O 2p π_\pm .

Values of exchange integrals J_σ and J_π , calculated from nodeless Slater functions, were obtained from Dr. M. Boyd³⁵ for the range 1.7 - 2.5 Å, and were extrapolated to 3 Å. Although these exchange integrals do not give the correct magnitude of the energy, it is assumed that their relative contributions are correct and given by their ratio $J^* = J_\pi/J_\sigma$. The ground state energy was rewritten as $J_\sigma (1 - \frac{3}{2} J^*)$. J_σ , now a parameter, was evaluated as a function of r , by equating $J_\sigma (1 - \frac{3}{2} J^*)$ to the ground state energy $V(r)$. The interaction energies for the excited states were then obtained, by evaluating the energy expressions in terms of $J_\sigma(r)$ and $J^*(r)$. (See Table 5 and Fig. 2). The methods described

earlier were used to obtain the potentials from which collision integrals are calculated.

As seen from the energy expressions, the $4\Sigma^-$ and 4Π states are coincident (in this approximation) and lie above the $2\Sigma^-$. All excited states are repulsive. The 4Π state would appear to be low by a factor of two (and the $2\Sigma^-$ too high by more) if the predissociation requirements were definitive. If the estimated curves are assumed good to a factor of 2, then the results suggest that $2\Sigma^-$ does not predissociate the $v = 2$ level of the A state, and the 4Π may indeed predissociate the $v = 8$ level. In order of increasing energy the states are given here as $2\Sigma^-$, 4Π , ($4\Sigma^-$). Note that this is contrary to the order given by Mulliken²⁷: 4Π , $4\Sigma^-$, $2\Sigma^-$.

V. RESULTS-CALCULATION OF COLLISION INTEGRALS AND TRANSPORT COEFFICIENTS

The details of the calculation procedure for obtaining collision integrals and transport coefficients are given in the work on hydrogen,¹ where all terms are defined. The expressions for the transport coefficients are those of the Chapman-Enskog first approximation.³⁶ For Li_2 and LiH the states considered are 1Σ and 3Σ ; for OH the states are $2\Pi_1$, $2\Sigma^-$, 4Π , and $4\Sigma^-$. The collision integrals, $\Omega^{(\ell,s)}$, were obtained for repulsive states from Monchick's³⁷ collision integrals for a repulsive exponential potential, and for the attractive states from Brokaw's³⁸ table of approximate collision integrals for an attractive exponential function.

Collision integrals for the Morse function, which can be written as

$$V(r) = \epsilon \left[e^{-\frac{2c(r-r_e)}{\sigma}} - 2e^{-\frac{c(r-r_e)}{\sigma}} \right], \quad (1)$$

have been tabulated by Lovell and Hirshfelder.³⁹ Here ϵ is the well depth at equilibrium separation r_e , σ is the value of r for $V=0$, and the parameter c is related to the width of the potential well. At sufficiently low reduced temperatures, $T^* = kT/\epsilon$, the repulsive part of the potential is negligible, and the collision integrals become those for an attractive exponential function. By determination of the scaling laws and intercomparison of the Morse function collision integrals, for different values of c , it was found that the tabulations were not given to low enough T^* to allow a check on the accuracy of Brokaw's approximate collision integrals for the attractive exponential function.

For the pairs of interacting species $\text{Li} + \text{Li}$, $\text{Li} + \text{H}$, and $\text{O} + \text{H}$, total collision integrals were obtained from a weighted average of the possible interaction states.⁴⁰ Table 6 lists the potential energy functions used for calculation of the collision integrals. The weights used were:

$\text{Li} + \text{Li}$: $^1\Sigma = 1/4$, $^3\Sigma = 3/4$; $\text{Li} + \text{H}$: $^1\Sigma = 1/4$, $^3\Sigma = 3/4$;

$\text{O} + \text{H}$: $^2\Pi_1 = 4/18$, $^2\Sigma = 2/18$, $^4\Sigma^- = 4/18$, $^4\Pi = 8/18$.

Spin degeneracy is included for all states, and orbital degeneracy⁴¹ for the Π states. The total collision integrals (weighted average) for $\text{Li} + \text{Li}$ are given in Table 7, for $\text{Li} + \text{H}$ in Table 8, and for $\text{O} + \text{H}$ in Table 9. In all cases considered, the greatest uncertainty

in the collision integrals comes from the estimated repulsive curves. Collision integrals for the $^1\Sigma$ state of Li_2 , $^1\Sigma$ state of LiH , and $^2\Pi$, $^2\Sigma^-$, $^4\Pi$, $^4\Sigma^-$ states of OH are given in the thesis of one of the authors (PHK).

Using these collision integrals, we obtain the transport coefficients in the temperature range of $1000^\circ\text{--}10,000^\circ\text{K}$. The diffusion coefficients are tabulated for a pressure of one atmosphere. For $\text{Li} + \text{H}$ mixtures the viscosity, translational thermal conductivity, and thermal diffusion factor are given in Tables 10, 11, and 12, respectively. For $\text{O} + \text{H}$ mixtures the corresponding transport coefficients are given in Tables 13, 14 and 15. Table 16 gives the diffusion coefficients, at one atmosphere pressure, for $\text{Li} + \text{Li}$, $\text{Li} + \text{H}$, and $\text{O} + \text{H}$.

Collision integrals and values of viscosity and conductivity for $\text{H} + \text{H}$ interactions were taken from Vanderslice, et al.^{1a} and the values for $\text{O} + \text{O}$ were from Yun and Mason.^{2a}

Wilke⁴² has given an approximate formula for obtaining η_{mix} from a knowledge of η_1 and η_2 at the temperature of interest. For a binary mixture the formula can be written as

$$\eta_{\text{mix}} \approx \frac{\eta_1}{1 + G_{12} \left(\frac{x_2}{x_1} \right)} + \frac{\eta_2}{1 + G_{21} \left(\frac{x_1}{x_2} \right)}, \quad (2)$$

$$G_{12} = \frac{1}{2\sqrt{2}} \left(\frac{M_2}{M_1 + M_2} \right)^{\frac{1}{2}} \left[1 + \left(\frac{\eta_1}{\eta_2} \right)^{\frac{1}{2}} \left(\frac{M_2}{M_1} \right)^{\frac{1}{4}} \right]^2, \quad (3)$$

where G_{21} is obtained from (3) by interchange of subscripts 1 and 2, or from

$$\frac{G_{12}}{G_{21}} = \frac{\eta_1 M_2}{\eta_2 M_1} . \quad (4)$$

A similar formula has been given by Mason and Saxena⁴³ for approximating λ_{mix} , with η replaced by λ in (2) but not in (3). Formulas of this general type have been used for many years (Sutherland-Wassiljewa formulas), and a large number of theoretical and semiempirical equations for G_{12} and G_{21} have been proposed. They have been recently critically reviewed and interpreted by Wright and Gray.⁴⁵ Several values of η_{mix} and λ_{mix} for a 1:1 mixture of Li + H and a 1:2 mixture O + H are calculated from the formulas of Wilke, and of Mason and Saxena (see Table 17), and found to be rather larger than the accurate values. One reason for the discrepancy is the fact that in the derivation of Eq. (3), the collision integral $(\bar{\Omega}_{12})^{\frac{1}{2}}$ is approximated by the arithmetic mean of $(\bar{\Omega}_{11})^{\frac{1}{2}}$ and $(\bar{\Omega}_{22})^{\frac{1}{2}}$. This is a fair approximation for valence-saturated atoms and molecules, but turns out to be rather poor for both Li+H and O + H. Indeed, for O + H the value of $\bar{\Omega}_{12}$ is greater than either $\bar{\Omega}_{11}$ or $\bar{\Omega}_{22}$.

For purposes of interpolation, formulas of the Sutherland-Wassiljewa type are convenient. One simple procedure is to write G_{12} and G_{21} in terms of a single empirical parameter Λ_{12} , first introduced by Mason and von Ubisch,⁴⁴

$$G_{12} = \frac{\lambda_1^0}{\Lambda_{12}} = \frac{15}{4} \frac{\eta_1}{M_1} \frac{R}{\Lambda_{12}} , \quad (5)$$

$$G_{21} = \frac{\lambda_2^0}{\Lambda_{12}} = \frac{15}{4} \frac{\eta_2}{M_2} \frac{R}{\Lambda_{12}} \quad (6)$$

The parameter Λ_{12} was obtained at each temperature by fitting the viscosity formula at the 50-50 composition to the exact results. The parameter R/Λ_{12} is given as a function of temperature in Table 18. This interpolation formula gives η_{mix} to within 1% of the accurate values for Li + H and O + H at all compositions. For λ_{mix} the approximate formula gives values larger than the exact, with deviations of up to 8% at low temperature and equimolar composition. The magnitude of these deviations is unusually large, showing that the G_{ij} are rather different for viscosity and thermal conductivity for these systems.

In fitting the semiempirical functions at long range by the potentials used to calculate the collision integrals, it was not necessary to have fitted two different repulsive potentials for diffusion and for conductivity, even though each property emphasizes a slightly different region of energies. Within the accuracy attainable, a single function would have sufficed.

VI. DISCUSSION

A. Potential Curves

(a) RKR Potential Curves

The RKR potentials for Li_2 , i.e., the classical turning points, are considered accurate to about one part in 10^3 . The greatest uncertainty is contributed by the extrapolation of the rotational constants beyond the range of rotational analysis.⁷

For the X state, rotational data were extrapolated beyond $v = 4$; for the B state a linear extrapolation of rotational data was made beyond $v = 1$. No extrapolation of data was made for the A and C states.

(b) Long-range Potentials

Since the long-range attractive potentials are extrapolated from fitted ground-state RKR curves, and the excited (repulsive) curves are obtained semiempirically, it is not possible to determine the absolute accuracy of the potentials obtained.

However, the discussions in Section III indicate that the estimated repulsive potentials may be uncertain by a factor of two at short range, and perhaps more at longer range. The attractive curves are probably accurate to within a few percent in the high temperature region, since they are short extrapolations of accurately known curves. At longer range, corresponding to the region of interest for lower temperatures, the extrapolation may lead to uncertainties in the potentials as large as 50%, or perhaps a factor of two. The repulsive curves for OH are estimated to be given to within a factor to two.

B. Collision Integrals and Transport Coefficients

In general, an error by a factor of two in the potential causes an error in the collision integrals of 20-40%. Greatest uncertainties in potentials occur at long range (i.e. low temperature), but these propagate less sensitively into the collision integrals, and give an overall estimate of uncertainty in the individual collision integrals of about 20-50%. However, the

total collision integrals are a weighted average of those for each state. For example: If, for OH, the $^4\Pi$ state were too low by a factor of two, and the $^2\Sigma^-$ state too high by a factor of ten, the total collision integrals would be too small by only 12%. This fortuitous near-cancellation indicates the importance of the weighting factor for each state.

A point worth noting is the extraordinarily large magnitude of the collision integrals for Li + Li and, though smaller, the relatively large size of the integrals for Li + H. That these integrals should have relatively large values is suggested by the wide potential well of the ground state of Li_2 . Making use of the Slater screening constants,⁴⁶ we can obtain a rough confirmation of the magnitude of the collision integrals. The collision diameter σ is given²³ by $\sigma = \bar{r}_a + \bar{r}_b + 1.8\text{\AA}$, where \bar{r} , the mean radius of an electron in the outer Slater orbital, is

$$\bar{r} = \frac{n^*(2n^*+1)(0.529)}{2(Z-S)}, \quad (7)$$

where Z is the atomic number, n^* the effective principal quantum number, and S the Slater screening constant. Since $\bar{\Omega} \approx \sigma^2$, we obtain $\bar{\Omega}(\text{Li} + \text{Li}) \approx 34.3\text{\AA}^2$, $\bar{\Omega}(\text{Li} + \text{H}) \approx 21.4\text{\AA}^2$, $\bar{\Omega}(\text{O} + \text{H}) \approx 10.0\text{\AA}^2$, which roughly confirm the values obtained more accurately.

For conditions when molecules and ions contribute significantly, the collision integrals for atom-atom interactions reported here are still necessary, though no longer sufficient for determining the transport coefficients.

The largest value of α_T for ordinary gas mixtures

previously reported⁴⁷ is 0.64, for a radon-helium mixture. For trace concentrations of Li in Li + H, especially at low temperatures, the value of α_T is very large (up to .97). Furthermore, the variation of α_T with composition at constant temperature is a factor of 5 from one end of the composition range to the other for Li + H, but only a factor of 2 for O + H. Both of these effects can be traced to the fact that the collision integrals for Li + Li collisions are so much larger than those for H + H collisions.

The diffusion coefficients of Li + Li, Li + H and H + H are roughly in the ratio 1:3:15. This again gives a measure of how large an atom of one species looks to itself and to an atom of another species. For Li + H, at low temperature, η_{mix} is relatively insensitive to change in composition for $x_1 > 0.5$, where x_1 is the mole fraction of Li in the mixture. The approximate formulas in Eqs. (2) and (3) indicate why this result should occur. Since $M_1/M_2 \approx 7$ and $\eta_2/\eta_1 \approx 3$, we find $G_{12} \ll G_{21}$, and thus for x_1/x_2 large the viscosity of the mixture is essentially that of Li atoms.

Svehla⁴⁸ gives values of viscosity and thermal conductivity for Li atoms, based on the use of a L-J(12-6) potential with the parameter ϵ/k estimated from boiling temperature and the parameter σ estimated from the molar volume at the boiling point. The ratio of his values to those reported here for η and λ^0 is about 2.2. Svehla considers only the molecular ground state in his calculations. Also, his arbitrary choice of potential and parameters ϵ/k and σ are less fundamentally based than the potentials given here. Therefore, his estimates of the transport coefficients are

considered less reliable than the results of the present calculation. In view of the crudeness of his assumptions and the uncertainties in the present calculations, the agreement appears as good as could be expected.

ACKNOWLEDGMENTS

The authors are grateful to Professor R. F. Barrow for sending them his experimental data on Li_2 prior to publication. They are also indebted to Dr. M. Klein and J. Hilsenrath of the National Bureau of Standards for the use of their computer programs, to Dr. Marjorie Boyd for information on the numerical values of the exchange integrals for OH, and especially to Professor S. Weissman of the Institute for Molecular Physics for programming the calculation of the transport coefficients.

Table 1. Potential energy of the $X^1\Sigma_g^+$ state of Li_2 .^{a, b}

v	$V(\text{cm}^{-1})$	$V(\text{ev})$	$r_{\min}(\text{\AA})$	$r_{\max}(\text{\AA})$
0	175.1	.0217	2.517	2.849
1	521.6	.0647	2.414	2.992
2	826.6	.1069	2.348	3.099
3	1199.	.1487	2.296	3.191
4	1530.	.1896	2.254	3.275
5	1855.	.2299	2.218	3.354
6	2174.	.2695	2.185	3.429
7	2488.	.3085	2.156	3.503
8	2796.	.3466	2.129	3.574
9	3099.	.3841	2.105	3.644
10	3396.	.4210	2.082	3.712
11	3687.	.4571	2.061	3.780
12	3973.	.4926	2.041	3.847
13	4254.	.5274	2.022	3.915
14	4526.	.5611	2.004	3.981

$$r_e = 2.6725 \text{ \AA}$$

a Data from references 9 and 10.

b Rotational data extrapolated beyond $v=4$.

Table 2. Potential energy of the $A^1\Sigma_u^+$ state of Li_2 .^a

v	$V(\text{cm}^{-1})$	$V(\text{ev})$	$T_e + V(\text{ev})$	$r_{\min}(\text{\AA})$	$r_{\max}(\text{\AA})$
0	127.3	.0158	1.7600	2.925	3.314
1	379.6	.0471	1.7913	2.805	3.482
2	628.8	.0780	1.8222	2.728	3.607
3	874.9	.1085	1.8527	2.669	3.714
4	1118.	.1386	1.8828	2.620	3.811
5	1358.	.1683	1.9125	2.578	3.902

$$T_e = 14068.36 \text{ cm}^{-1} = 1.7442 \text{ ev}$$

$$r_e = 3.1077 \text{ \AA}$$

a Data from reference 10.

Table 3. Potential energy of the $B^1\Pi_u$ state of $Li_2^{a,b}$

v	$V(\text{cm}^{-1})$	$V(\text{ev})$	$T_e + V(\text{ev})$	$r_{\min}(\text{\AA})$	$r_{\max}(\text{\AA})$
0	134.2	.0166	2.5506	2.761	3.139
1	398.8	.0494	2.5834	2.645	3.308
2	656.4	.0814	2.6154	2.572	3.436
3	907.9	.1126	2.6466	2.515	3.549
4	1153.	.1430	2.6770	2.468	3.653
5	1390.	.1723	2.7063	2.428	3.751
6	1620.	.2009	2.7349	2.390	3.851
7	1843.	.2284	2.7624	2.356	3.948
8	2057.	.2550	2.7890	2.325	4.043
9	2264.	.2805	2.8145	2.296	4.138
10	2457.	.3047	2.8387	2.262	4.249
11	2642.	.3276	2.8616	2.232	4.355
12	2817.	.3493	2.8833	2.203	4.461
13	2978.	.3692	2.9032	2.176	4.568

$$T_e = 20439.4 \text{ cm}^{-1} = 2.5340 \text{ ev}$$

$$r_e = 2.9364 \text{ \AA}$$

a Data from references 9, 11, 12, and 13.

b Rotational data extrapolated beyond $v=1$.

Table 4. Potential energy of the $C^1\Pi_u$ state of Li_2 .^a

v	$V(\text{cm}^{-1})$	$V(\text{ev})$	$T_e + V(\text{ev})$	$r_{\min}(\text{\AA})$	$r_{\max}(\text{\AA})$
0	118.2	.0146	3.8021	2.894	3.298
1	349.6	.0433	3.8308	2.774	3.482
2	575.0	.0713	3.8588	2.699	3.623
3	794.6	.0985	3.8860	2.641	3.748
4	1009.0	.1251	3.9126	2.595	3.861
5	1218.0	.1510	3.9385	2.554	3.969
6	1423.0	.1764	3.9639	2.519	4.074

$$T_e = 30549.9 \text{ cm}^{-1} = 2.7875 \text{ ev}$$

$$r_e = 3.0750 \text{ \AA}$$

a Data from references 14 and 15.

Table 5. Electronic states of OH.

State	Configuration	Exchange energy
4_{Σ^-}	$\sigma^2 \pi_+ \pi_- \sigma^*$	$- 2J_{\pi} - J_{\sigma}$
4_{Π}	$\sigma \pi^2 \pi_+ \pi_- \sigma^*$	$- 2J_{\pi} - J_{\sigma}$
2_{Σ^+}	$\sigma^2 \pi_+ \pi_- \sigma^*$	$+ J_{\pi} - J_{\sigma}$
2_{Π_1}	$\sigma^2 \pi_+^2 \pi_-$	$- \frac{3}{2} J_{\pi} + J_{\sigma}$

Table 6. Potential energy functions used for calculation of collision integrals.

System	State	Potential energy (cm^{-1}) (r in Å)	Transport Coefficient	Range of r (Å)
Li + Li	3Σ	$2.997 \times 10^5 e^{-r/1.0076}$	viscosity	3.8-6.5
	3Σ	$5.125 \times 10^5 e^{-r/0.9157}$	diffusion	3-5.5
	1Σ	$-2.021 \times 10^5 e^{-r/1.0708}$	diffusion & viscosity	4-7
Li + H	3Σ	$1.066 \times 10^6 e^{-r/0.6334}$	viscosity	3.25-5
	3Σ	$7.415 \times 10^5 e^{-r/0.6700}$	diffusion	2.75-4.85
	1Σ	$-9.138 \times 10^5 e^{-r/0.6443}$	diffusion & viscosity	3.5-5
O + H	2Π	$-8.837 \times 10^5 e^{-r/0.3807}$	diffusion & viscosity	1.2-3
	2Σ	$1.136 \times 10^6 e^{-r/0.3708}$	diffusion & viscosity	1.7-2.8
	$4\Pi, 4\Sigma$	$1.784 \times 10^6 e^{-r/0.3669}$	diffusion & viscosity	1.9-2.9

Note: Within the accuracy attainable, the repulsive states of Li_2 and LiH could have been fitted by a single function for both diffusion and viscosity, which depend on different regions of the potential.

Table 7. Weighted average collision integrals and ratios in \AA^2 .

Li + Li

T °K	$\bar{\Omega}^{(1,1)}$	$\bar{\Omega}^{(2,2)}$	A*	B*	C*
1000	33.96	40.05	1.179	1.196	0.892
1500	29.69	34.86	1.174	1.207	0.886
2000	26.85	31.38	1.169	1.215	0.881
2500	24.76	28.81	1.163	1.222	0.876
3000	23.13	26.78	1.158	1.228	0.873
3500	21.79	25.13	1.153	1.234	0.870
4000	20.67	23.74	1.148	1.238	0.867
4500	19.72	22.54	1.143	1.243	0.865
5000	18.88	21.50	1.139	1.247	0.862
5500	18.14	20.56	1.133	1.251	0.860
6000	17.48	19.73	1.129	1.254	0.858
6500	16.89	18.98	1.124	1.258	0.856
7000	16.34	18.30	1.120	1.261	0.854
7500	15.85	17.68	1.115	1.264	0.853
8000	15.40	17.10	1.111	1.266	0.851
8500	14.99	16.57	1.106	1.269	0.849
9000	14.61	16.08	1.101	1.273	0.848
9500	14.24	15.62	1.097	1.275	0.847
10000	13.91	15.19	1.092	1.277	0.846

Table 8. Weighted average collision integrals and ratios in \AA^2 .

Li + H

T $^{\circ}\text{K}$	$\bar{\Omega}^{(1,1)}$	$\bar{\Omega}^{(2,2)}$	A_{12}^*	B_{12}^*	C_{12}^*
1000	19.92	22.98	1.153	1.180	0.902
1500	17.64	20.54	1.164	1.191	0.896
2000	16.11	18.89	1.172	1.198	0.892
2500	14.97	17.65	1.179	1.204	0.888
3000	14.06	16.67	1.185	1.209	0.884
3500	13.33	15.86	1.190	1.214	0.881
4000	12.71	15.18	1.194	1.218	0.879
4500	12.17	14.59	1.198	1.222	0.877
5000	11.71	14.07	1.202	1.225	0.874
5500	11.29	13.61	1.205	1.228	0.872
6000	10.92	13.19	1.208	1.232	0.870
6500	10.58	12.82	1.211	1.234	0.868
7000	10.28	12.47	1.214	1.237	0.867
7500	10.00	12.16	1.216	1.240	0.865
8000	9.74	11.87	1.219	1.242	0.864
8500	9.50	11.59	1.221	1.244	0.862
9000	9.28	11.34	1.223	1.246	0.861
9500	9.07	11.10	1.225	1.248	0.859
10000	8.88	10.88	1.226	1.250	0.858

Table 9. Weighted average collision integrals and ratios in O_2 .

O + H

T °K	$\bar{\Omega}^{(1,1)}$	$\bar{\Omega}^{(2,2)}$	A_{12}^*	B_{12}^*	C_{12}^*
1000	7.337	8.507	1.159	1.168	0.910
1500	6.558	7.640	1.165	1.176	0.904
2000	6.032	7.053	1.169	1.182	0.900
2500	5.640	6.614	1.173	1.188	0.897
3000	5.309	6.243	1.176	1.192	0.894
3500	5.075	5.977	1.178	1.196	0.892
4000	4.858	5.733	1.180	1.200	0.890
4500	4.673	5.521	1.182	1.204	0.888
5000	4.510	5.336	1.183	1.206	0.886
5500	4.364	5.170	1.185	1.209	0.884
6000	4.234	5.022	1.186	1.212	0.883
6500	4.116	4.886	1.187	1.214	0.881
7000	4.008	4.764	1.189	1.217	0.880
7500	3.910	4.650	1.189	1.219	0.879
8000	3.817	4.544	1.190	1.221	0.877
8500	3.733	4.447	1.191	1.222	0.876
9000	3.654	4.356	1.192	1.225	0.875
9500	3.581	4.270	1.193	1.226	0.874
10000	3.512	4.191	1.193	1.229	0.873

Table 10. Viscosity of Li + H mixtures in millipoise
 (1 millipoise = 10^{-3} g/cm-sec)

T°K	mole fraction of Li atoms					
	0	0.2	0.4	0.6	0.8	1.0
1000	.142	.0877	.0703	.0624	.0581	.0555
1500	.199	.121	.0975	.0870	.0814	.0781
2000	.253	.153	.124	.111	.104	.100
2500	.305	.184	.149	.134	.126	.122
3000	.356	.215	.174	.157	.148	.144
3500	.407	.244	.198	.179	.170	.166
4000	.453	.273	.223	.202	.192	.187
4500	.498	.302	.247	.225	.214	.209
5000	.542	.329	.270	.247	.236	.231
5500	.586	.358	.294	.270	.259	.254
6000	.633	.386	.318	.292	.281	.276
6500	.682	.415	.343	.315	.304	.299
7000	.732	.444	.367	.338	.326	.321
7500	.782	.473	.391	.361	.349	.344
8000	.832	.501	.415	.384	.372	.368
8500	.881	.530	.439	.407	.395	.391
9000	.931	.559	.464	.431	.418	.415
9500	.981	.588	.488	.454	.442	.439
10000	1.03	.617	.513	.478	.466	.463

Table 11. Translational thermal conductivity of Li + H mixtures
in millicalories/cm-sec-°K.

T°K	mole fraction of Li atoms					
	0	0.2	0.4	0.6	0.8	1.0
1000	1.05	0.457	0.256	0.157	0.0980	0.0596
1500	1.47	0.637	0.357	0.219	0.137	0.0839
2000	1.87	0.810	0.454	0.278	0.175	0.108
2500	2.26	0.978	0.548	0.336	0.212	0.131
3000	2.64	1.14	0.641	0.394	0.248	0.154
3500	3.01	1.31	0.733	0.450	0.285	0.178
4000	3.35	1.46	0.823	0.506	0.321	0.201
4500	3.68	1.62	0.912	0.562	0.357	0.225
5000	4.00	1.77	0.999	0.617	0.393	0.248
5500	4.33	1.92	1.09	0.673	0.430	0.272
6000	4.68	2.08	1.18	0.730	0.466	0.296
6500	5.04	2.24	1.27	0.785	0.503	0.321
7000	5.41	2.40	1.36	0.842	0.540	0.345
7500	5.78	2.56	1.45	0.898	0.577	0.370
8000	6.15	2.72	1.54	0.955	0.614	0.395
8500	6.52	2.88	1.63	1.01	0.651	0.420
9000	6.89	3.04	1.72	1.07	0.688	0.445
9500	7.26	3.20	1.81	1.12	0.726	0.471
10,000	7.63	3.36	1.90	1.18	0.764	0.497

Table 12. Thermal diffusion factor α_T for Li + H mixtures.

T°K	mole fraction of Li atoms					
	0	0.2	0.4	0.6	0.8	1.0
1000	0.97	0.52	0.35	0.27	0.22	0.18
1500	0.89	0.47	0.32	0.25	0.20	0.17
2000	0.84	0.44	0.30	0.23	0.18	0.16
2500	0.79	0.41	0.28	0.21	0.17	0.14
3000	0.73	0.38	0.26	0.20	0.16	0.13
3500	0.69	0.36	0.24	0.19	0.15	0.13
4000	0.66	0.34	0.23	0.18	0.14	0.12
4500	0.62	0.33	0.22	0.17	0.14	0.12
5000	0.58	0.30	0.21	0.16	0.13	0.11
5500	0.54	0.29	0.20	0.15	0.12	0.10
6000	0.52	0.27	0.19	0.14	0.12	0.096
6500	0.49	0.26	0.18	0.14	0.11	0.091
7000	0.48	0.25	0.17	0.13	0.10	0.088
7500	0.45	0.24	0.16	0.12	0.099	0.083
8000	0.44	0.23	0.16	0.12	0.096	0.080
8500	0.41	0.22	0.15	0.11	0.090	0.075
9000	0.40	0.21	0.14	0.11	0.086	0.072
9500	0.37	0.19	0.13	0.099	0.080	0.067
10 000	0.36	0.18	0.13	0.095	0.077	0.065

Table 13. Viscosity of O + H mixtures in millipoise
 (1 millipoise = 10^{-3} g/cm-sec)

T°K	mole fraction of O atoms					
	0	0.2	0.4	0.6	0.8	1.0
1000	0.142	0.247	0.325	0.384	0.432	0.470
1500	0.199	0.339	0.441	0.519	0.580	0.630
2000	0.253	0.425	0.550	0.644	0.718	0.778
2500	0.305	0.508	0.653	0.763	0.849	0.917
3000	0.356	0.589	0.755	0.878	0.974	1.05
3500	0.407	0.667	0.851	0.988	1.09	1.18
4000	0.453	0.742	0.946	1.10	1.21	1.31
4500	0.498	0.816	1.04	1.20	1.33	1.43
5000	0.542	0.889	1.13	1.31	1.44	1.55
5500	0.586	0.961	1.22	1.41	1.55	1.67
6000	0.633	1.03	1.31	1.51	1.66	1.78
6500	0.682	1.11	1.40	1.61	1.77	1.90
7000	0.732	1.18	1.49	1.71	1.88	2.01
7500	0.782	1.25	1.58	1.81	1.99	2.12
8000	0.832	1.33	1.66	1.91	2.09	2.24
8500	0.881	1.40	1.75	2.01	2.20	2.35
9000	0.931	1.47	1.84	2.10	2.30	2.46
9500	0.981	1.54	1.92	2.20	2.40	2.56
10,000	1.03	1.62	2.01	2.29	2.51	2.67

Table 14. Translational thermal conductivity of O + H mixtures
in millicalories/cm-sec- $^{\circ}$ K

T° K	mole fraction of O atoms					
	0	0.2	0.4	0.6	0.8	1.0
1000	1.05	0.720	0.511	0.373	0.280	0.219
1500	1.47	1.00	0.706	0.512	0.381	0.293
2000	1.87	1.26	0.891	0.644	0.476	0.362
2500	2.26	1.53	1.07	0.771	0.567	0.427
3000	2.64	1.78	1.25	0.896	0.655	0.489
3500	3.01	2.03	1.42	1.01	0.739	0.549
4000	3.35	2.26	1.58	1.13	0.823	0.608
4500	3.68	2.49	1.75	1.25	0.905	0.665
5000	4.00	2.72	1.91	1.36	0.986	0.721
5500	4.33	2.95	2.07	1.48	1.07	0.776
6000	4.68	3.18	2.23	1.59	1.15	0.830
6500	5.04	3.42	2.39	1.70	1.22	0.884
7000	5.41	3.66	2.56	1.82	1.30	0.938
7500	5.78	3.91	2.72	1.93	1.38	0.990
8000	6.15	4.15	2.89	2.05	1.46	1.04
8500	6.52	4.39	3.05	2.16	1.54	1.09
9000	6.89	4.63	3.22	2.27	1.61	1.15
9500	7.26	4.87	3.38	2.38	1.69	1.19
10,000	7.63	5.12	3.55	2.50	1.77	1.24

Table 15. Thermal diffusion factor α_T for O + H mixtures.

T°K	mole fraction of O atoms					
	0	0.2	0.4	0.6	0.8	1.0
1000	0.45	0.37	0.32	0.28	0.25	0.22
1500	0.42	0.35	0.30	0.26	0.23	0.20
2000	0.40	0.33	0.28	0.24	0.21	0.19
2500	0.39	0.32	0.27	0.23	0.20	0.18
3000	0.37	0.30	0.26	0.22	0.20	0.18
3500	0.36	0.29	0.25	0.21	0.19	0.17
4000	0.35	0.28	0.24	0.21	0.18	0.16
4500	0.34	0.27	0.23	0.20	0.18	0.16
5000	0.32	0.26	0.22	0.19	0.17	0.15
5500	0.31	0.25	0.21	0.18	0.16	0.14
6000	0.31	0.25	0.21	0.18	0.16	0.14
6500	0.30	0.24	0.20	0.17	0.15	0.14
7000	0.29	0.24	0.20	0.17	0.15	0.13
7500	0.29	0.23	0.19	0.17	0.15	0.13
8000	0.28	0.22	0.19	0.16	0.14	0.13
8500	0.27	0.22	0.18	0.16	0.14	0.12
9000	0.27	0.21	0.18	0.15	0.13	0.12
9500	0.26	0.21	0.17	0.15	0.13	0.12
10 000	0.26	0.20	0.17	0.15	0.13	0.11

Table 16. Diffusion coefficients of Li + Li, Li + H, and O + H.

T, °K	D_{ij} (1 atm), cm^2/sec		
	Li + Li	Li + H	O + H
1000	0.929	3.14	8.22
1500	1.95	6.52	16.9
2000	3.32	11.0	28.3
2500	5.04	16.5	42.3
3000	7.09	23.2	59.1
3500	9.48	30.8	77.9
4000	12.2	39.4	99.4
4500	15.3	49.1	123.
5000	18.7	59.8	150.
5500	22.4	71.5	178.
6000	26.5	84.3	209.
6500	31.0	98.1	243.
7000	35.8	113.	279.
7500	40.9	129.	317.
8000	46.4	146.	358.
8500	52.2	163.	401.
9000	58.3	182.	446.
9500	64.9	202.	493.
10 000	71.7	223.	543.

Table 17(a). Approximate values of η_{mix} and λ_{mix} for a 1:1 mixture of Li + H.

T °K	η_{mix} (millipoise)	% Dev	λ_{mix} (millical/cm-sec-°K)	% Dev
1000	0.0717	+ 8.6	0.247	+24
5000	0.294	+14.4	0.999	+28
10000	0.582	+18.3	1.966	+34

Table 17(b). Approximate values of η_{mix} and λ_{mix} for a 1:2 mixture of O + H.

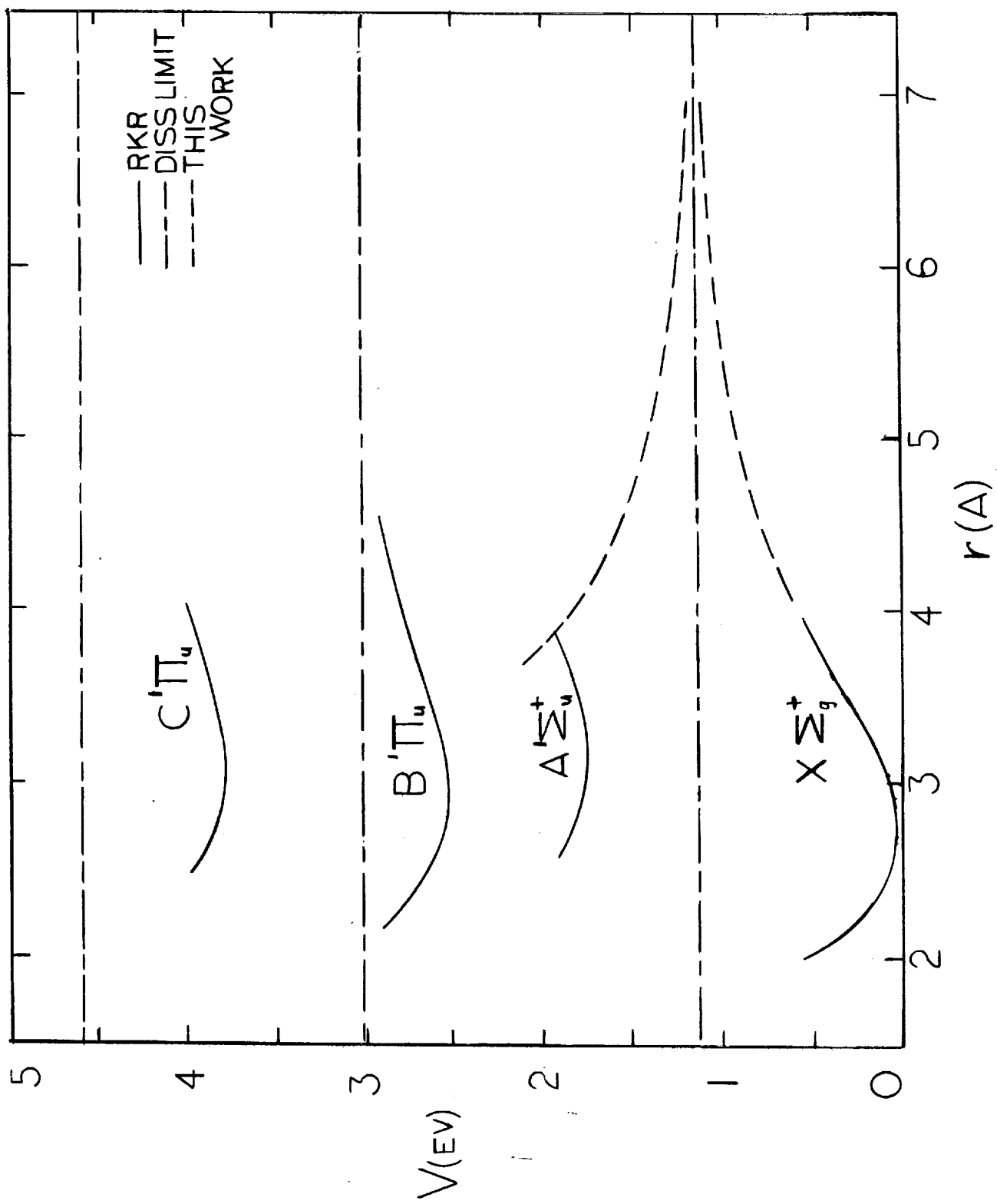
T °K	η_{mix} (millipoise)	% Dev	λ_{mix} (millical/cm-sec-°K)	% Dev
1000	0.369	+23	0.733	+28
5000	1.274	+20	2.657	+24
10000	2.264	+20	4.898	+22

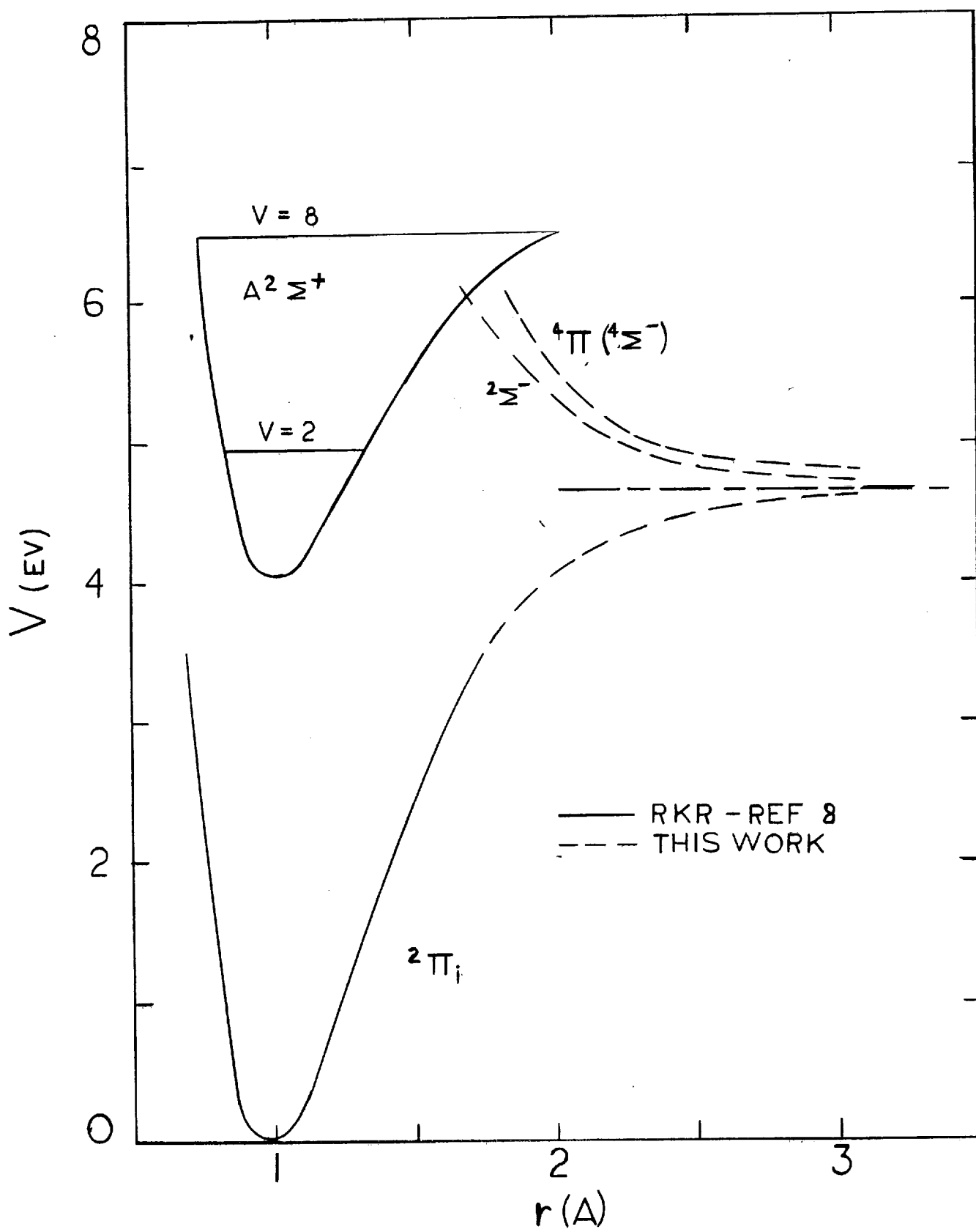
Table 18. Interpolation factor for approximate
calculation of η_{mix} and λ_{mix} .

T°K	$\frac{R}{\Lambda_{12}} \quad \frac{\text{cm-sec}}{\text{mole}}$	
	Li + H	O + H
1000	9863	4500
1500	7204	3282
2000	5741	2613
2500	4802	2185
3000	4142	1876
3500	3653	1660
4000	3270	1487
4500	2965	1349
5000	2716	1235
5500	2505	1139
6000	2326	1058
6500	2172	988
7000	2038	927
7500	1919	873
8000	1815	825
8500	1721	782
9000	1636	744
9500	1560	709
10,000	1490	678

Fig. 1. Potential energy curves for Li_2 .

Fig. 2. Long-range potentials for OH.





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